

# Spin nematic fluctuations near a spin-density-wave phase

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**Abstract.** We study an interacting electronic system exhibiting a spin nematic instability. Using a phenomenological form for the spin fluctuation spectrum near the spin-density-wave (SDW) phase, we compute the spin nematic susceptibility in energy and momentum space as a function of temperature and the magnetic correlation length  $\xi$ . The spin nematic instability occurs when  $\xi$  reaches a critical value  $\xi_{\text{cr}}$ , i.e., its transition temperature  $T_{\text{SN}}$  is always higher than the SDW critical temperature  $T_{\text{SDW}}$ . In particular,  $\xi_{\text{cr}}$  decreases monotonically with increasing  $T_{\text{SN}}$ . Concomitantly, low-energy nematic fluctuations are present in a wider temperature region as  $T_{\text{SN}}$  becomes higher. Approaching the spin nematic instability, the nematic spectral function at zero momentum exhibits a central peak as a function of energy for a finite temperature and a soft mode at zero temperature. These properties originate from the general feature that the imaginary part of the spin-fluctuation bubble has a term linear in energy and its coefficient is proportional to the square of temperature. Furthermore we find that the nematic spectral function exhibits a diffusive peak around zero momentum and zero energy without clear dispersive features. A possible phase diagram for the spin nematic and SDW transitions is also discussed.

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## 1. Introduction

The mechanism of high-temperature superconductivity is one of the major issues in condensed matter physics. By carrier doping into antiferromagnetic Mott insulators, cuprate superconductors attain high critical temperatures  $T_c$ , typically of more than 77 K, the boiling temperature of liquid nitrogen at ambient pressure. Since it is widely accepted that doped cuprates can be described within a one-band model it is natural to assume that the important fluctuations are spin fluctuations in these systems. In 2008 another family of high- $T_c$  superconductors was discovered consisting of iron-based pnictides [1]. Similar to the cuprate case, superconductivity occurs close to a magnetic

phase. However, in contrast to the cuprates, the magnetic phase is metallic and several bands cross the Fermi energy, suggesting the importance of orbital degrees of freedom. Thus there are two different kinds of fluctuations in the pnictides which may be relevant for their physical properties, namely, spin and orbital fluctuations.

In general it is not easy to assess the relative importance of the two kinds of fluctuations in observable quantities. It is known that superconducting order parameters due to spin fluctuations tend to have  $s_{\pm}$  symmetry [2, 3] whereas those due to orbital fluctuations have  $s_{++}$  symmetry [4, 5]. While this difference in the gap symmetries can contribute to identifying the underlying mechanism of superconductivity, a recent theoretical study [6] shows that  $s_{\pm}$  pairing gap can be stabilized even for orbital fluctuations when a partial contribution from spin fluctuations is taken into account. Experimentally the superconducting phase occurs often closer to the nematic than to the magnetic phase [7, 8, 9]. From this one may conclude that nematic fluctuations play also an important role for superconductivity and more generally for the physics of pnictides. It is thus important to study the properties of nematic fluctuations and their origin in detail.

The nematic instability is accompanied by a structural phase transition from a tetragonal to an orthorhombic phase. This structural phase transition is believed to be driven by the coupling to electronic degrees of freedom [8], because the observed anisotropy of resistivity [10], the optical conductivity [11] and the splitting of electronic bands [12] is much larger than what one would expect from the lattice anisotropy. Due to these effects the orthorhombic phase in the pnictides, which breaks the  $C_4$  symmetry of the normal state, is referred to as an electronic nematic phase. Depending on the electronic degrees of freedom responsible for the nematicity, three kinds of nematicity can be distinguished: charge [13, 14, 15, 16], orbital [17, 18], and spin nematicity [19]. For iron-based pnictides, the latter two possibilities seem to be relevant.

Orbital nematicity in pnictides is associated with a spontaneous difference in the occupation of  $d_{yz}$  and  $d_{zx}$  orbitals [20, 21, 22]. Below the transition temperature the orientational symmetry is broken, whereas all the other symmetries remain unbroken. Orbital fluctuations may lead to a superconducting state driven mainly by fluctuations around zero momentum [4]. In this scenario, nesting of the Fermi surfaces is not crucial for pairing. Orbital fluctuations around a finite momentum [23, 5] may, similarly to spin fluctuations [2, 3], also lead to superconductivity but in this case nesting properties of the Fermi surface are important. Considering general orbital fluctuations, retardation effects and quasi-particle weights within Eliashberg theory it was shown [24] that orbital nematic fluctuations produce strong coupling superconductivity. The obtained transition temperatures and the fact that superconductivity also occurs inside the nematic phase are compatible with the experimental observations.

Spin nematicity in iron-based pnictides is associated with a spontaneous anisotropy of the spin fluctuation spectrum in momentum space between  $(\pi, 0)$  and  $(0, \pi)$  [25, 26]. Spin nematicity owes its existence to spin fluctuations and is caused by the interaction between them as reviewed in [27] and [28]. It has the general property that it can occur

above the spin-density-wave (SDW) phase [27], which is in nice agreement with the experimental findings.

In general it is difficult to distinguish between spin and orbital nematicity because there is a coupling between the corresponding order parameters. If the orbital (spin) nematic instability occurs, the spin (orbital) nematic order is induced via a linear coupling between them [28]. Hence both orbital and spin nematic orders occur always at the same time. Nevertheless, one may argue that the original instability occurs only in the orbital or the spin section. As a result one mechanism will dominate and it makes sense to study the two kinds of mechanisms leading to the nematic state independently.

Using linear response theory we will investigate in this paper properties near the spin nematic instability. The results are rather independent of microscopic details because the functional form for the spin fluctuation propagator becomes generic close to the SDW phase. The characteristic features of the low-energy spin nematic fluctuations are determined by the anomalous asymptotic behavior of the spin fluctuation bubble at low frequencies. Our results for the dynamic structure factor are predictions which can be checked by inelastic light scattering. We also present a schematic phase diagram containing spin nematic and magnetic transition temperatures.

## 2. Model and formalism

The spin nematicity in iron-based superconductors can be formulated in terms of an action as in [29]. Here we wish to formulate it in terms of a conventional operator formalism and to clarify the diagrammatic structure of spin nematic physics.

Iron-based superconductors are often described by a five-band Hubbard model [3]. To describe the spin nematic interaction in a microscopic model, we focus on the effective interaction of the total spin operator. Then our microscopic model consists of electrons hopping between the sites of a square lattice and interacting via their total spins. The corresponding Hamiltonian becomes

$$H = \sum_{\mathbf{k}, \alpha, \sigma} \epsilon_{\mathbf{k}\alpha} c_{\mathbf{k}, \alpha, \sigma}^\dagger c_{\mathbf{k}, \alpha, \sigma} + \frac{1}{2N} \sum_{\mathbf{q}} J(\mathbf{q}) \mathbf{S}(\mathbf{q}) \cdot \mathbf{S}(-\mathbf{q}), \quad (1)$$

with the total spin operator

$$\mathbf{S}(\mathbf{q}) = \frac{1}{2} \sum_{\mathbf{k}, \alpha, \sigma, \sigma'} c_{\mathbf{k}, \alpha, \sigma}^\dagger \boldsymbol{\tau}_{\sigma\sigma'} c_{\mathbf{k}+\mathbf{q}, \alpha, \sigma'}. \quad (2)$$

$c_{\mathbf{k}, \alpha, \sigma}^\dagger$  creates an electron in the band  $\alpha$  with spin direction  $\sigma$ , and  $c_{\mathbf{k}, \alpha, \sigma}$  annihilates this electron.  $\boldsymbol{\tau}$  is the vector of the three Pauli matrices,  $\epsilon_{\mathbf{k}\alpha}$  the one-particle energies of the band  $\alpha$ ,  $J(\mathbf{q})$  the strength of the spin-spin interaction in momentum space, and  $N$  is the total number of the lattice sites.

Besides the total spin operator we will consider the spin nematic operator

$$\Phi(\mathbf{q}) = \frac{1}{\sqrt{2}N} \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \mathbf{S}(\mathbf{k} + \mathbf{q}/2) \cdot \mathbf{S}(-\mathbf{k} + \mathbf{q}/2). \quad (3)$$

$\gamma_{\mathbf{k}}$  is equal to one if  $\mathbf{k}$  is close to  $(\pi, 0)$  or  $(-\pi, 0)$  and equal to minus one if  $\mathbf{k}$  is close to  $(0, \pi)$  or  $(0, -\pi)$ .  $\gamma_{\mathbf{k}}$  has  $d$ -wave symmetry and the sum over  $\mathbf{k}$  in Eq. (3) runs over the entire Brillouin zone (BZ).

The dynamic spin susceptibility is defined by

$$\chi(\mathbf{q}, \omega) = \frac{i}{N} \int_0^\infty dt \langle [\mathbf{S}_l(\mathbf{q}, t), \mathbf{S}_l(-\mathbf{q}, 0)] \rangle e^{i\omega t}, \quad (4)$$

where the index  $l$  denotes a Cartesian component,  $[\cdot, \cdot]$  the commutator, and  $\omega$  includes tacitly a small imaginary part  $i\eta$ ; we consider a state with spin rotational symmetry and thus  $\chi$  does not depend on  $l$ . In a similar way we define a spin nematic susceptibility by

$$\chi_{\text{SN}}(\mathbf{q}, \omega) = \frac{i}{N} \int_0^\infty dt \langle [\Phi(\mathbf{q}, t), \Phi(-\mathbf{q}, 0)] \rangle e^{i\omega t}. \quad (5)$$

Going over to the Matsubara representation, the usual diagrammatic perturbation expansion for electronic systems holds for the above two correlation functions. Concerning  $\chi(\mathbf{q}, \omega)$  we are interested in the following in its low-frequency and long-wavelength behavior. Here long-wavelength means momenta near  $(\pi, 0)$  or  $(0, \pi)$  or the equivalent points in the BZ. Thus we do not try to calculate  $\chi$  by a perturbation expansion but expand the inverse susceptibility in powers of  $\omega$  and  $\mathbf{q} - \mathbf{Q}_{\mathbf{q}}$  where  $\mathbf{Q}_{\mathbf{q}}$  denotes  $(\pi, 0)$  for  $\mathbf{q}$  close to  $(\pi, 0)$  and  $(0, \pi)$  for  $\mathbf{q}$  close to  $(0, \pi)$ . The result is

$$\chi(\mathbf{q}, \omega) = \frac{c/\gamma}{r + (\mathbf{q} - \mathbf{Q}_{\mathbf{q}})^2 - i\omega/\gamma}. \quad (6)$$

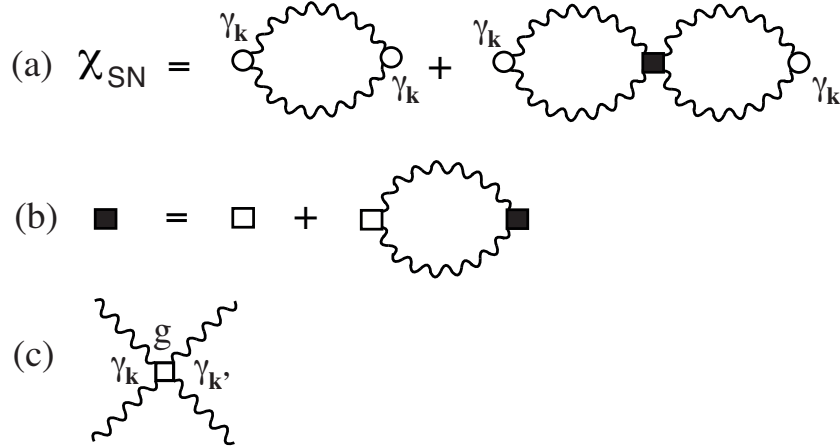
$r$  is equal to  $1/\xi^2$  where  $\xi$  is the correlation length.  $\gamma$  is a damping constant and  $c$  determines the spectral weight. The above parametrization of  $\chi$  is a general form of spin fluctuations near the SDW phase and in fact describes rather well the measured imaginary part of the spin susceptibility in  $\text{BaFe}_{1.85}\text{Co}_{0.15}\text{As}_2$  by choosing appropriate parameters [30].

The lowest order diagrams for the evaluation of  $\chi_{\text{SN}}$  are shown in figure 1(a). The wavy line stands for the spin propagator  $-\chi$ , i.e., for a two-particle propagator. The first diagram represents  $\chi_{\text{SN}}^{(0)}$  for the non-interacting case, whereas the second term comes from the spin nematic interaction. The effective interaction (solid square) represents the four-spin vertex as shown in figures 1(b) and (c). The open square denotes a ring diagram where the sides of the square represent electronic Green's functions and the corner points of the square the interaction term in Eq. (1). Taking the low-frequency, long-wavelength limit in external spin legs the four-spin vertex collapses to one constant  $g$ . The effective interaction term assumes then the form

$$H_I = -\frac{g}{2N} \sum_{\mathbf{q}} \Phi(\mathbf{q}) \Phi(-\mathbf{q}). \quad (7)$$

The resulting diagrams for  $\chi_{\text{SN}}$  are shown in Fig. 1. Altogether one obtains

$$\chi_{\text{SN}}(\mathbf{q}, \omega) = \frac{\chi_{\text{SN}}^{(0)}(\mathbf{q}, \omega)}{1 - g\chi_{\text{SN}}^{(0)}(\mathbf{q}, \omega)}. \quad (8)$$



**Figure 1.** Graphical representation of the spin nematic susceptibility  $\chi_{\text{SN}}$ . The wavy line indicates spin fluctuations and the vertex with a circle in (a) represents a form factor  $\gamma_{\mathbf{k}}$  associated with the spin nematic order parameter [see (3)]. The solid square is an effective four-point vertex of spin fluctuations defined in (b). The open square in (b) and (c) is a bare four-point vertex of spin fluctuations due to the spin nematic interaction [see (7)].

The analytic expression for  $\chi_{\text{SN}}^{(0)}$  is

$$\chi_{\text{SN}}^{(0)}(\mathbf{q}, i\omega_n) = \frac{3T}{N} \sum_{\mathbf{k}, m} \chi(\mathbf{k} + \mathbf{q}/2, i\omega_n + i\nu_m) \chi(-\mathbf{k} + \mathbf{q}/2, -i\nu_m), \quad (9)$$

where  $\omega_n$  and  $\nu_m$  are bosonic Matsubara frequencies, the factor 3 comes from spin rotational symmetry and  $T$  is the temperature. In the long-wavelength and low-frequency limit follows from the above equation for small  $r$ ,

$$\chi_{\text{SN}}^{(0)}(\mathbf{0}, 0) = \frac{3T}{N} \sum_{\mathbf{k}, m} [\chi(\mathbf{k}, i\nu_m)]^2 > \frac{3T}{N} \sum_{\mathbf{k}} [(\chi(\mathbf{k}, 0))]^2 \sim \frac{T}{r}. \quad (10)$$

Assuming  $g$  to be positive [attractive interaction in (7)], (10) implies that  $\chi_{\text{SN}}(\mathbf{0}, 0)$  will diverge at a finite temperature for a finite and positive  $r$  independently how large the coupling constant  $g$  is. This means that a nematic transition will always take place before the long-range magnetic phase at  $r = 0$  is reached if  $g$  is positive and  $T$  finite.

In order to evaluate Eq. (9) we use the spectral representation for  $\chi$ ,

$$\chi(\mathbf{q}, i\omega_n) = \int_{-\infty}^{\infty} d\epsilon \frac{A(\mathbf{q}, \epsilon)}{i\omega_n - \epsilon}, \quad (11)$$

with

$$A(\mathbf{q}, \epsilon) = -\frac{c}{\pi\gamma} \frac{\epsilon/\gamma}{[r + (\mathbf{q} - \mathbf{Q}_{\mathbf{q}})^2]^2 + \epsilon^2/\gamma^2}. \quad (12)$$

Inserting (11) into (9) and carrying out the frequency sum yields after an analytic continuation for the imaginary part

$$\text{Im } \chi_{\text{SN}}^{(0)}(\mathbf{q}, \omega) = \frac{3\pi}{N} \sum_{\mathbf{k}} \int_{-\infty}^{\infty} d\epsilon A(\mathbf{k} + \mathbf{q}/2, \epsilon + \omega) A(-\mathbf{k} + \mathbf{q}/2, \epsilon) [n(\epsilon) - n(\omega + \epsilon)], \quad (13)$$

with  $n(\epsilon) = 1/(e^{\epsilon/T} - 1)$ . The real part of  $\chi_{\text{SN}}^{(0)}$  is computed via a Kramers-Kronig relation,

$$\text{Re}\chi_{\text{SN}}^{(0)}(\mathbf{q}, \omega) = \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{\infty} d\nu \frac{\text{Im}\chi_{\text{SN}}^{(0)}(\mathbf{q}, \nu)}{\nu - \omega}, \quad (14)$$

where p.v. denotes the principal value. The function  $\chi_{\text{SN}}(\mathbf{q}, \omega)$  is then obtained from (8), (13) and (14). The spectral function of the spin nematic fluctuations is given by

$$S(\mathbf{q}, \omega) = \frac{1}{\pi} [1 + n(\omega)] \text{Im}\chi_{\text{SN}}(\mathbf{q}, \omega), \quad (15)$$

which we compute numerically.

### 3. Results

#### 3.1. Choice of parameters

To compute the spin nematic spectrum numerically from (8) and (9), we first fix the spin fluctuation propagator [see (6)] and the coupling strength  $g$  [see (7)]. Neutron scattering data [30] for  $\text{BaFe}_{1.85}\text{Co}_{0.15}\text{As}_2$  yield parameters for the spin fluctuation spectrum, namely,  $c \approx 1.3$  and  $\gamma \approx 230$  meV. Hence we take in the present theory

$$c = 1 \quad \text{and} \quad \gamma = 1, \quad (16)$$

measuring all quantities with the dimension of energy in units of  $\gamma$ . For the mass term  $r$  we take in the normal state

$$r = r_{\text{cr}} + (T - T_{\text{SN}}) \quad \text{for} \quad T \geq T_{\text{SN}}. \quad (17)$$

The bare susceptibility  $\chi_{\text{SN}}^{(0)}(\mathbf{0}, 0)$  depends on  $T$  and  $r$ . The instability equation of the normal state with respect to the nematic state [see (8)],

$$1 = g\chi_{\text{SN}}^{(0)}(\mathbf{0}, 0), \quad (18)$$

yields a relation between the critical mass  $r_{\text{cr}} = r(T_{\text{SN}})$  and the nematic transition temperature  $T_{\text{SN}}$ . The value of  $T_{\text{SN}}$  (or equivalently  $r_{\text{cr}}$ ) can be considered as a free parameter and we will study the spin nematic spectrum for various choices of  $T_{\text{SN}}$ . At  $T = 0$ , (17) is not valid and  $r$  should be taken as a non-thermal control parameter, for example, concentration of an isovalent substitution, carrier density, or pressure.

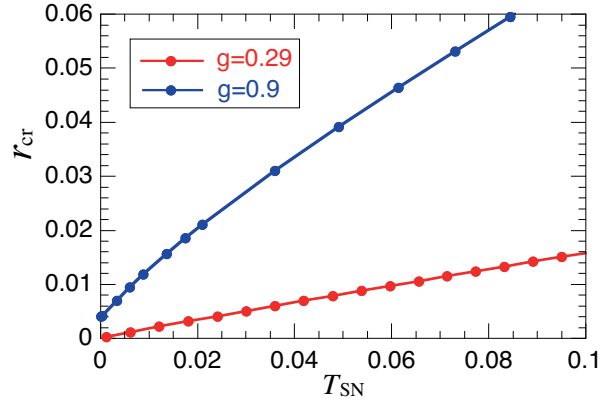
According to the phase diagram of  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  in [31], a structural phase transition and the SDW instability occur at 80 K and 70 K, respectively, at  $x = 0.04$ . If the structural phase transition is assumed to be associated with the spin nematic instability, the present theory reproduces the experimental transition temperatures at  $x = 0.04$  for  $g = 0.29$ , extrapolating  $r$  linearly down to  $T_{\text{SDW}}$ . Since a different value of  $g$  would be obtained if one considers experimental data at a different  $x$ , we will also take  $g = 0.9$  later to clarify how our results depend on the choice of  $g$ .

We first study the case of  $g = 0.29$ , and calculate the critical value  $r_{\text{cr}}$  as a function of  $T_{\text{SN}}$  (figure 2) and the spectral weight of spin nematic fluctuations in  $\mathbf{q}$  and  $\omega$  space (figures 3, 4, and 5). We will then consider results for a larger coupling strength  $g = 0.9$

(figures 2, 6, and 7). On the basis of these results, we sketch typical phase diagrams of the spin nematic phase near the SDW phase (figure 8).

### 3.2. Numerical results

We put  $\mathbf{q} \rightarrow \mathbf{0}$  and  $\omega \rightarrow 0$  in (8) and study the spin nematic instability. We search for its onset temperature  $T_{\text{SN}}$  by determining the temperature at which  $\chi_{\text{SN}}(\mathbf{0}, 0)$  diverges for a given  $r_{\text{cr}}$ . Figure 2 shows  $r_{\text{cr}}$  as a function of  $T_{\text{SN}}$  for two coupling strengths  $g$ .  $r_{\text{cr}}$  is always positive and increases with increasing  $T_{\text{SN}}$ . This feature can easily be understood by using the approximate expression (10) for  $\chi_{\text{SN}}^{(0)}$  which holds at large temperatures. The instability condition Eq. (18) becomes then equivalent to  $r_{\text{cr}} \sim gT_{\text{SN}}$ . The linear dependence of  $r_{\text{cr}}$  with  $T_{\text{SN}}$  is at least approximately reflected in the calculated curves in figure 2. The same holds for the increase of the slope with increasing  $g$ .

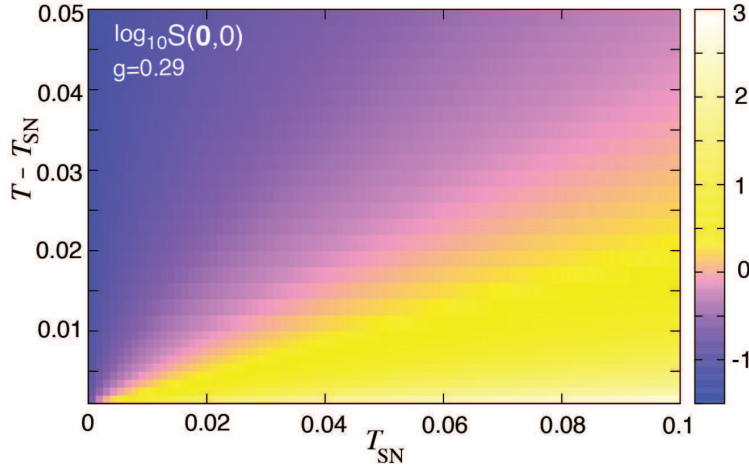


**Figure 2.** (Color online) Critical value  $r_{\text{cr}}$  as a function of the onset temperature of the spin nematic instability  $T_{\text{SN}}$  for a spin nematic coupling strength of  $g = 0.29$  and  $0.9$ .

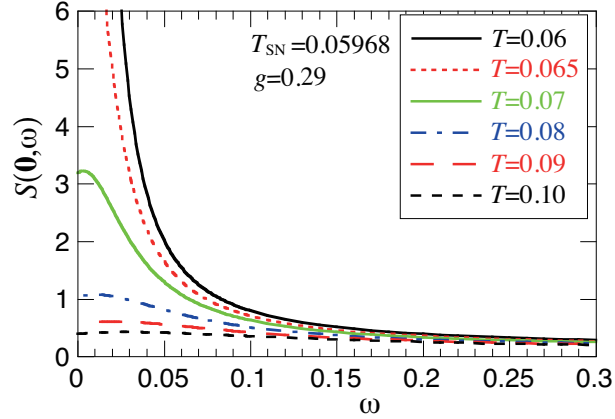
Figure 3 shows the spectral weight of the spin nematic fluctuations at  $\mathbf{q} = \mathbf{0}$  and  $\omega = 0$  in the plane of  $T_{\text{SN}}$  and  $T - T_{\text{SN}}$ . The spectral weight is enhanced upon approaching  $T_{\text{SN}}$  and eventually diverges at  $T_{\text{SN}}$ . In particular, strong fluctuations appear at higher temperatures above  $T_{\text{SN}}$  if  $T_{\text{SN}}$  becomes larger, as seen in the yellow region in figure 3. For  $T_{\text{SN}} \approx 0$ , on the other hand, the enhancement of the spectral weight occurs only very close to  $T = T_{\text{SN}}$ .

Retaining still  $\mathbf{q} = \mathbf{0}$ , we next present in figure 4 the dependence of the spectral weight on  $\omega$  for several temperatures. At high temperature well above  $T_{\text{SN}}$  the spectrum is almost flat at low energies and its weight is very small. With decreasing temperature the low-energy spectral weight is enhanced to form a peak at zero energy in form of a central peak. This peak grows more and more upon approaching  $T_{\text{SN}}$  and finally diverges at  $T_{\text{SN}}$ .

Figure 5 is a  $\mathbf{q}$ - $\omega$  map of the spectral weight near the spin nematic instability. The highest spectral weight is located around  $\mathbf{q} = \mathbf{0}$  and  $\omega = 0$  and the weight spreads



**Figure 3.** (Color online) Spectral weight of the spin nematic fluctuations at  $\mathbf{q} = \mathbf{0}$  and  $\omega = 0$  for  $g = 0.29$  in the plane of  $T_{\text{SN}}$  and  $T - T_{\text{SN}}$ ; the spectral weight is plotted on a logarithmic scale.

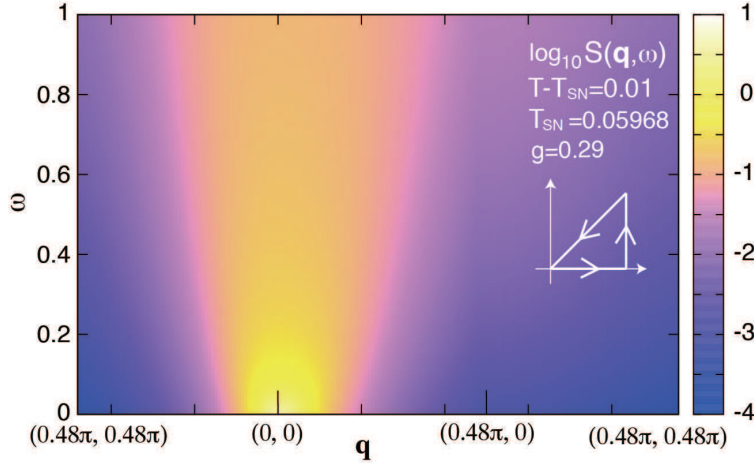


**Figure 4.** (Color online)  $\omega$  dependence of the spectral weight at  $\mathbf{q} = \mathbf{0}$  for  $g = 0.29$  and different temperatures. The spin nematic instability occurs at  $T_{\text{SN}} = 0.05968$  with the critical value  $r_{\text{cr}} = 0.00968$ .

with increasing energy while its strength is decreasing, like the tail of a comet. That is, the spin nematic fluctuations appear as a diffusive peak around  $\mathbf{q} = \mathbf{0}$  and  $\omega = 0$ , and no dispersive features can be seen. While we have chosen  $T_{\text{SN}} = 0.05968$  and  $T - T_{\text{SN}} = 0.01$  in figure 5, essentially the same result is obtained for other choices of parameters, although the *tail of the comet* is gradually blurred with increasing  $T$ .

We next comment on results at  $T_{\text{SN}} = 0$ . Figure 2 shows that for the coupling strength  $g = 0.29$   $r_{\text{cr}}$  almost vanishes at  $T_{\text{SN}} = 0$ . Hence the spin nematic and SDW instability occur almost simultaneously. Collective effects of spin nematic fluctuations occur only in the vicinity of  $T = T_{\text{SN}}$  as can be inferred from figure 3. As a result spin nematic fluctuations are enhanced only well below  $T \approx 10^{-4}$  for  $T_{\text{SN}} = 0$ . If a larger value for the coupling strength  $g$  is used, spin nematic fluctuations for  $T_{\text{SN}} = 0$  become

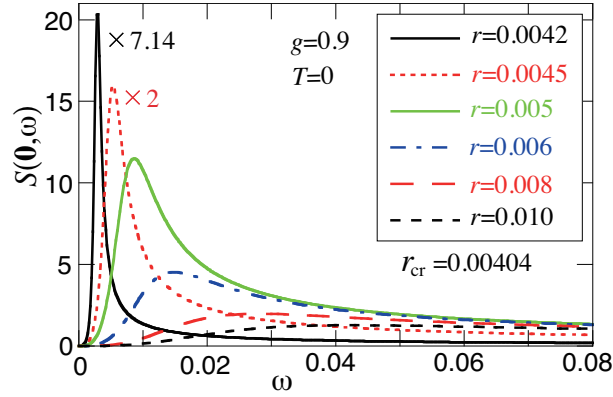




**Figure 5.** (Color online)  $\mathbf{q}$ - $\omega$  map of the spectral weight on a logarithmic scale for  $g = 0.29$ . The scanned direction of  $\mathbf{q}$  is sketched inside the figure:  $(0.48\pi, 0.48\pi) \rightarrow (0, 0) \rightarrow (0.48\pi, 0) \rightarrow (0.48\pi, 0.48\pi)$ . The spectrum has a fourfold symmetry in momentum space above  $T_{\text{SN}}$ .

visible at much higher temperatures. For  $g = 0.9$ , for instance, the overall temperature scale associated with the spin nematic instability becomes much larger than for  $g = 0.29$  and low-energy fluctuations are strongly enhanced already below  $T \approx 0.02$  [ $\approx 50$  K, see (16) and also figure 7]. We have checked also that there is no qualitative change in figures 3, 4, and 5 if a finite  $T_{\text{SN}}$  is considered and  $g$  is increased from 0.29 to 0.9.

At zero temperature we consider  $r$  in (6) as a non-thermal control parameter, see also the statement below (18). We plot in figure 6 the  $\omega$  dependence of the spin nematic spectral weight at  $\mathbf{q} = \mathbf{0}$  for several values of  $r$  above the spin nematic instability at  $r_{\text{cr}} = 0.00404$  for  $g = 0.9$ . In contrast to the case of a finite  $T$ , described in figure 4, no central peak is formed and the weight at  $\omega = 0$  remains zero when approaching the spin nematic instability. Instead spin nematic fluctuations appear as a soft mode. With decreasing  $r$  a peak structure forms at a finite energy and moves towards lower frequencies. When  $r$  approaches  $r_{\text{cr}}$ , the width of the peak becomes very narrow and at the same time the height of the peak increases strongly. At the spin nematic transition  $r = r_{\text{cr}}$  the weight diverges at  $\omega = 0$ . The presence of the soft mode suggests that there might be a dispersive feature of the spin nematic fluctuations in the plane of  $\mathbf{q}$  and  $\omega$  at zero temperature. Hence we computed maps of the spectral weight, similar to figure 5, at  $T = 0$ . The dispersive feature is actually obtained, but only for  $r$  very close to  $r_{\text{cr}}$ ; furthermore it becomes visible only in the vicinity of  $\mathbf{q} = \mathbf{0}$  and  $\omega = 0$ , on a much smaller scale than that in figure 5. In this sense, the dispersive feature is extremely weak. In fact, once  $r$  becomes a little larger than  $r_{\text{cr}}$ , spin nematic fluctuations produce a diffusive signal around  $\mathbf{q} = \mathbf{0}$  and  $\omega = 0$  even at  $T = 0$ , similar as in figure 5.



**Figure 6.** (Color online)  $\omega$  dependence of the spin nematic spectral weight at  $\mathbf{q} = \mathbf{0}$  for several values of  $r$ . The weights for  $r = 0.0045$  and  $0.0042$  are actually larger by a factor 2 and 7.14, respectively, as indicated in the figure.

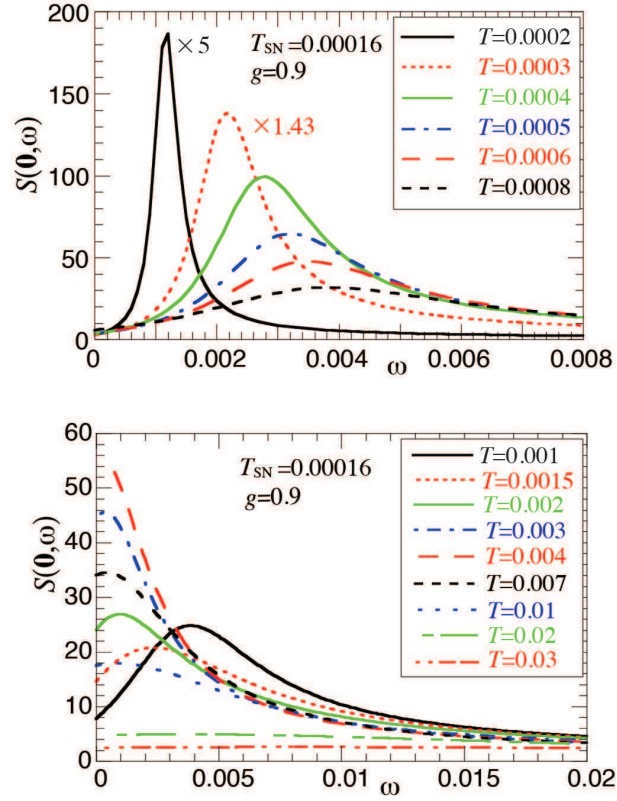
### 3.3. Asymptotic behavior of $\chi_{\text{SN}}^{(0)}$ at low frequencies

Our obtained results can easily be understood by analyzing the low-energy property of the spin-fluctuation bubble  $\chi_{\text{SN}}^{(0)}(\mathbf{q}, \omega)$ . From (13) follows  $\text{Im}\chi_{\text{SN}}^{(0)}(\mathbf{q}, -\omega) = -\text{Im}\chi_{\text{SN}}^{(0)}(\mathbf{q}, \omega)$ , i.e.,  $\text{Im}\chi_{\text{SN}}^{(0)}(\mathbf{q}, \omega)$  is an odd function of the frequency. Evaluating (13) for  $\omega, T \ll r$  yields the asymptotic expansion

$$\text{Im}\chi_{\text{SN}}^{(0)}(\mathbf{0}, \omega) \propto \frac{T^2}{r^3} \omega + a_3 \omega^3 + \dots, \quad (19)$$

where  $a_3$  is a constant. There is a term linear in  $\omega$ , which yields a central peak as found in figure 4. Its coefficient has a  $T^2$  dependence, leading in figure 3 to strong fluctuations over a wide temperature region above  $T_{\text{SN}}$  for a higher  $T_{\text{SN}}$ . On the other hand, at  $T = 0$ , the linear term vanishes and the spectral weight is characterized by  $\omega^3$  at low  $\omega$ , leading to a substantial suppression of the spin nematic fluctuations at low  $\omega$ . This is the reason why spin nematic fluctuations are strongly suppressed at low temperatures (figure 3) and no central peak is present. Instead a soft mode associated with spin nematic fluctuations occurs at  $T = 0$  as shown in figure 6. Since the spin-fluctuation propagator is in general parameterized by (6) close to the SDW instability, the low-energy dependence of (19) is understood as a general feature of the spin-fluctuation bubble. This low-energy property yields characteristic features of the spin nematic fluctuations found in figures 3 - 6 as well as the spin nematic instability close to the SDW phase shown in figure 2.

The peculiar behavior of  $\chi_{\text{SN}}^{(0)}(\mathbf{0}, \omega)$  can be seen most clearly in figure 7. The two diagrams in this figure show the evolution of the spectral weight for  $g = 0.9$  as a function of temperature.  $T_{\text{SN}}$  is equal to 0.00016 and thus very small, yielding spectra which are also representative for  $T_{\text{SN}} = 0$ . Fixing  $T_{\text{SN}}$  means that also  $r_{\text{cr}}$  is fixed, see (17) and figure 2. The lower diagram shows that for  $T \gtrsim 0.02$  the spectrum is completely flat and structureless. Decreasing  $T$  down to 0.004 the spectral weight shifts towards lower frequencies and a central peak is formed. In this temperature range the linear term in  $\omega$  of  $\text{Im}\chi_{\text{SN}}^{(0)}(\mathbf{0}, \omega)$  still dominates in a low frequency expansion of  $\text{Im}\chi_{\text{SN}}^{(0)}$  [see (19)]



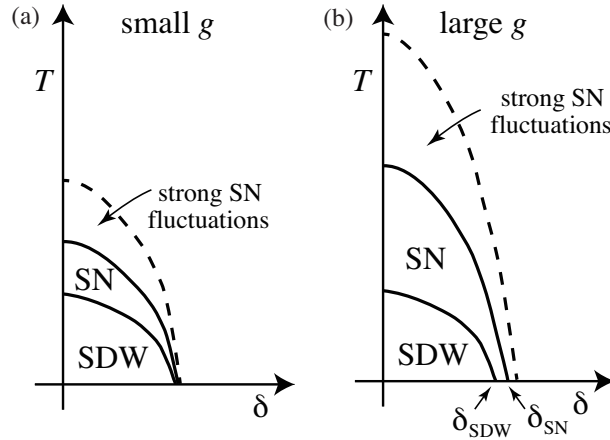
**Figure 7.** (Color online) Evolution of the spectral weight for  $g = 0.9$  and  $T_{\text{SN}} = 0.00016$  as a function of temperature. The critical value  $r_{\text{cr}}$  is 0.00406 (see figure 2).

and causes the central peak. Lowering further  $T$  to 0.001 the low frequency part of the spectral weight loses intensity and a propagating peak appears with an increasing frequency and a decreasing half-width. In this temperature interval the linear term in  $\omega$  of  $\text{Im}\chi_{\text{SN}}^{(0)}(\mathbf{0}, \omega)$ , proportional to  $T^2$ , becomes small and the term  $a_3\omega^3$  starts to play a role. As a result a transition from a diffusive to a propagating mode behavior is obtained. Considering the upper diagram and decreasing further the temperature the energy of the propagating peak and its half-width decrease whereas its height increases strongly.

### 3.4. Schematic phase diagram

On the basis of our obtained results (figures 2 and 3), we can infer a typical phase diagram for the spin nematic and SDW phases. Let the onset temperature of the SDW instability evolve as a function of a control parameter  $\delta$ , as shown in figure 8(a);  $\delta$  may correspond to the concentration of substituted ions, carrier density, pressure, or other quantities depending on material properties.  $T_{\text{SDW}}$  decreases with increasing  $\delta$  and vanishes at a critical value of  $\delta_{\text{SDW}}$ . Let us introduce the slope  $\alpha = r_{\text{cr}}/(T_{\text{SN}} - T_{\text{SDW}})$  ( $> 0$ ) and assume that  $\alpha$  depends only weakly on  $\delta$ . Approximating the results in figure 2 by  $r_{\text{cr}} \propto T_{\text{SN}}$ , we obtain  $T_{\text{SN}} - T_{\text{SDW}} \propto T_{\text{SDW}}$ , i.e., the temperature region

occupied by the spin nematic phase increases with increasing  $T_{\text{SDW}}$ . In the opposite limit where  $T_{\text{SDW}}$  is close to zero, i.e.,  $\delta \rightarrow \delta_{\text{SDW}}$ , the spin nematic phase vanishes very close to  $\delta_{\text{SDW}}$ . As seen from figure 3, the temperature region where strong spin nematic fluctuations are present expands for a higher  $T_{\text{SN}}$  and shrinks substantially near  $\delta_{\text{SDW}}$  as shown by the dashed line in figure 8(a). On the other hand, if the strength of the spin nematic interaction becomes very strong, the spin nematic phase as well as the region where strong spin nematic fluctuations are present expands to a larger region as shown in figure 8(b). In particular, a region of the spin nematic phase can be well separated from the SDW instability at zero temperature (see also figure 2 for  $g = 0.9$ ) and thus two well-separated quantum phase transitions exist as a function of  $\delta$ .



**Figure 8.** Schematic phase diagram of the spin nematic (SN) instability near the SDW phase on the plane of a control parameter  $\delta$  and the temperature for a realistic value of  $g$  for iron pnictides (left figure) and for a large  $g$  (right figure). The phase transition is assumed to be continuous. Two quantum phase transition occur at  $\delta_{\text{SN}}$  and  $\delta_{\text{SDW}}$ , and these two almost coincide for a small  $g$ .

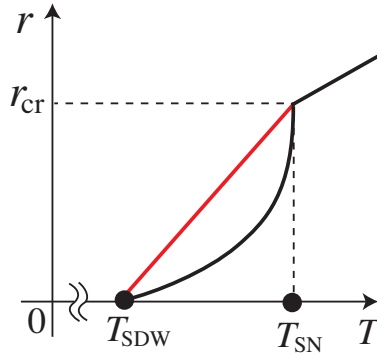
## 4. Discussions

### 4.1. Origin of the nematic phase in iron-based superconductors

We discuss the origin of the nematic phase observed in iron-based superconductors [8]. In figure 8, we assumed that  $T_{\text{SDW}}$  decreases monotonically with increasing  $\delta$ , which is the usual case in iron-based superconductors. The spin nematic scenario then predicts that the temperature difference of  $T_{\text{SN}}$  and  $T_{\text{SDW}}$ , namely  $r_{\text{cr}}/\alpha = T_{\text{SN}} - T_{\text{SDW}} > 0$ , should decrease monotonically with increasing  $\delta$ , at least, if  $\alpha$  depends only weakly on  $\delta$ . However, this tendency is not observed in iron-based superconductors in spite of the fact that many different compounds [7] have been investigated. We discuss several possibilities to resolve this qualitative discrepancy between the expectation and the experiment.

First, we have assumed a constant coupling strength  $g$  and a constant value of  $c$ ; the latter controls the overall strength of spin fluctuations [see (6)]. If  $g$  (and/or  $c$ ) is substantially suppressed at a low  $\delta$ ,  $T_{\text{SN}}$  would shift closer to  $T_{\text{SDW}}$  similar to the experimental observation. However, a theoretical study [29] suggests that the value of  $g$  becomes larger with decreasing  $\delta$ , so that  $r_{\text{cr}}$  is expected to be larger than in figure 8 at low  $\delta$ . The discrepancy between the present theory and experimental observations would even increase. In addition, the value of  $c$  is expected to become larger for a lower  $\delta$  because the nesting condition of the Fermi surfaces for the momenta  $(\pi, 0)$  and  $(0, \pi)$  becomes better at a lower  $\delta$ . Consequently, a more realistic treatment of  $g$  and  $c$  would lead to a larger discrepancy between theory and experiment.

Below  $T_{\text{SN}}$  the spin nematic order parameter  $\phi(T) (\geq 0)$  becomes nonzero. As a result  $r(T)$  has the form  $r^{(0)}(T) \pm \phi(T)$  where  $r^{(0)}(T)$  is equal to  $r_{\text{cr}} + (T - T_{\text{SN}})$  in agreement with the expression (17) in the normal state. The temperature dependence of  $r$  will approximately be given by the solid curve in figure 9. The sudden drop of  $r$  just below  $T_{\text{SN}}$  is due to the development of the spin nematic order parameter characterized by  $\phi(T) \sim (T_{\text{SN}} - T)^\beta$ ;  $\beta = 1/2$  in mean-field theory and  $\beta = 1/8$  in a two-dimensional system. The red line in figure 9 is a linear interpolation through the points  $(T, r) = (T_{\text{SN}}, r_{\text{cr}})$  and  $(T_{\text{SDW}}, 0)$  with the slope  $\alpha$ . The absolute value of  $\alpha$  simply changes the scale of temperature and thus is not relevant to the present discussion as long as  $\alpha$  is independent of  $\delta$ .



**Figure 9.** (Color online) Temperature dependence of  $r = \xi^{-2}$  ( $\xi$  is the magnetic correlation length) in the actual system (solid curve) and in the linear approximation (red line). The values of  $T_{\text{SN}}$ ,  $T_{\text{SDW}}$  and  $r_{\text{cr}}$  are correctly captured in the linear approximation, although the whole temperature dependence of  $r$  is not. The slope of the red line corresponds to  $\alpha$  and is assumed to depend weakly on  $\delta$  in figure 8.

To reconcile the observed nematic phase in terms of the spin nematic instability, we have to invoke a  $\delta$  dependence of  $\alpha$ . In the so-called "1111" compounds  $\text{LaFeAsO}_{1-x}\text{F}_x$  [32] and  $\text{CeFeAsO}_{1-x}\text{F}_x$  [33] the onset temperature of the nematic phase largely extends to the superconducting region even though the SDW state has already vanished. A similar feature is observed also for  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  [31], where the nematic phase is confined closer to the SDW phase as compared to the "1111" compounds. To understand

these data,  $\alpha$  must be assumed to become very large near  $x \approx 0$  so that  $T_{\text{SDW}}$  occurs much closer to  $T_{\text{SN}}$ . It also should decrease substantially with increasing  $x$  so that  $T_{\text{SDW}}$  occurs further away from  $T_{\text{SN}}$ . This  $\delta$  dependence should be so dramatic that it fully changes the qualitative features of the phase diagram (figure 8) and also compensate the possible further discrepancy caused by a realistic treatment of  $g$  and  $c$ . While the actual SDW transition changes to first order close to  $x = 0$  whereas the nematic transition is continuous there [34], such a region is rather small and thus does not modify our major discussion. In typical hole-doped compounds  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$  [35, 36] and isovalent doping materials  $\text{Ba}(\text{Fe}_{1-x}\text{Ru}_x)_2\text{As}_2$  [37, 38] the nematic phase occurs simultaneously with the SDW instability within experimental resolutions. To understand this,  $\alpha$  should be assumed to be very large near  $x = 0$  and to remain rather large with increasing  $x$ .

At present it is not clear whether the assumption of a  $\delta$  dependence of  $\alpha$  is justified from a microscopic point of view. To evaluate  $\alpha$  the absolute value of  $\phi(T)$  does matter as a function of  $T$  and moreover an approximation scheme to calculate  $r$  also does matter since  $r$  becomes zero only at  $T = 0$  in a purely two-dimensional system. Because of these subtleties in determining the precise form of the spin nematic phase, it seems natural to expect a substantial material dependence of the shape of the spin nematic region in the  $\delta$ - $T$  plane. Thus one would naturally expect a phase diagram similar to figure 8 at least for a certain class of materials if the spin nematicity is responsible for the nematic phase in iron-based superconductors in general. At present, however, no iron-based superconductors are known to show characteristic features of the spin nematicity shown in figure 8 [7]. Fernandes *et al.* study a possible phase diagram of the spin nematic phase near the SDW phase [29]. Their calculations are done in two limits: the zero-temperature limit and the classical limit in the sense that only the zero Matsubara frequency is considered in gap equations. Their results at  $T = 0$  predict that the spin nematic and SDW instabilities occur simultaneously. This is consistent with our results, although they predict a first order transition, a possibility which is not considered in our analysis. At finite temperatures they obtain in the classical limit figures 8 and 14 in [29] which compare successfully with experimental data and also present a microscopic treatment of the slope  $\alpha$ . In our approach all Matsubara frequencies are kept but  $\alpha$  is considered as a phenomenological input.

Our schematic phase diagram (figure 8) does not apply to the orbital nematic scenario, because the orbital nematic instability is controlled by a fermionic bubble diagram [39, 24]. Hence it is tempting to state that in general orbital nematicity is likely responsible for the nematic phase observed in iron-based superconductors [8, 7]. However, it seems too early to reach such a conclusion. In view of the fact that the nematic phase occurs in general close to the SDW phase, it is important to clarify from a microscopic point of view why this should also hold for the orbital nematic state. One possible reason is given in [5] where Kontani *et al.* point out the important role of Aslamazov-Larkin type diagrams. It is interesting to explore further whether the orbital nematic scenario indeed explains the fact that the nematic instability occurs close to the SDW phase at  $\delta = 0$  and the nematic region extends to a larger region with decreasing

$T_{\text{SDW}}$  and higher  $\delta$  as observed in experiments [7, 8, 9].

The iron-based superconductor FeSe shows a structural phase transition from an orthorhombic to a tetragonal phase with decreasing temperature, but no SDW phase has been detected [40]. This experimental fact naturally suggests that orbital nematicity is responsible for the structural phase transition. If we wish to understand the structural phase transition in FeSe in terms of the spin nematic order, we would invoke, for example, a large coupling strength  $g$ , as shown in the right panel in figure 8. FeSe would then be located in the region  $\delta_{\text{SDW}} < \delta < \delta_{\text{SN}}$ .

#### 4.2. Nematic fluctuations

Spin nematic fluctuations can be measured directly by electronic Raman scattering. Although the computation of the Raman intensity in a microscopic model for electrons is beyond the scope of the present study, our obtained spectra can be interpreted as  $B_{1g}$  Raman spectra within the following approximation. In a microscopic calculation the vertex  $\gamma_{\mathbf{k}}$  in figure 1(a) is replaced by a triangle diagram constructed from three electronic Green's functions. Such a triangle diagram depends both on momentum and frequency. Expanding its momentum dependence in terms of a complete set of functions with  $B_{1g}$  symmetry it is evident that only the function  $\gamma(\mathbf{k})$  contributes substantially due to the restriction of the momenta to the neighborhood of  $(\pi, 0)$  and  $(0, \pi)$ . Concerning the frequency it is plausible that the triangle diagram has no resonances at low frequencies in the range of collective nematic fluctuations. Thus the triangle diagram may be approximated by a constant and we expect that our results in figures 3-7 capture the major features of electronic Raman scattering due to spin nematic fluctuations in the  $B_{1g}$  channel. Although available Raman scattering data [41, 42, 43] are interpreted in terms of orbital nematic fluctuations [39], they do not seem to exclude the spin nematic scenario. Not only further theoretical studies but also more detailed experimental data are important to determine the origin of the nematic phase observed in iron-based superconductors. A crucial test to identify the origin of the nematic phase is to measure nematic fluctuations at zero temperature by suppressing the superconductivity, for example, by applying a large magnetic field: spin nematic fluctuations appear as a soft mode upon approaching the nematic phase whereas orbital fluctuations form a central peak.

We finally discuss a possible role of nematic fluctuations for superconductivity. If the nematic phase in iron-based superconductors is associated with spin nematicity, one might wonder about superconductivity mediated by spin nematic fluctuations. As shown in figures 3 and 8, spin nematic fluctuations are substantially suppressed at low temperatures. It is thus unlikely that such fluctuations are responsible for the observed superconductivity. Instead usual spin fluctuations provide a more natural scenario to understand superconductivity [2, 3] in these systems even if the spin nematic phase occurs in actual materials. On the other hand, if the nematic phase originates from orbital degrees of freedom, it has been shown that orbital nematic fluctuations can

lead to strong coupling superconductivity [24] in pnictides and thus provide an exotic mechanism for superconductivity in these systems.

## 5. Conclusions

Using a general form for the spin-fluctuation spectrum near the SDW phase we have studied spin nematic spectra in energy and momentum space. If the spin nematic interaction is attractive and the nematic transition continuous, its transition temperature  $T_{\text{SN}}$  is always higher than that to the antiferromagnetic state at  $T_{\text{SDW}}$ . The spin nematic spectra are characterized by several generic features: (i) the critical magnetic correlation length  $\xi_{\text{cr}}$  decreases with increasing  $T_{\text{SN}}$  (figure 2), (ii) strong low-energy spin nematic fluctuations extend to a wider temperature region for a larger  $T_{\text{SN}}$  (figure 3), (iii) the spin-nematic spectrum at  $\mathbf{q} = \mathbf{0}$  exhibits a central peak as a function of  $\omega$  close to the spin nematic instability at a finite temperature (figures 4 and 7) whereas it shows a soft mode upon approaching the spin nematic instability close to zero temperature (figures 6 and 7), and (iv) there is no clear dispersive mode associated with spin nematic fluctuations and instead a diffusive peak is obtained around  $\mathbf{q} = \mathbf{0}$  and  $\omega = 0$  (figure 5). These general features originate from the low-energy property of the simple bubble diagram of spin fluctuations [see (19)]. The resulting phase diagram is shown in figure 8 if  $\alpha$ , the average slope of  $r_{\text{cr}} = \xi_{\text{cr}}^{-2}$  as a function of temperature between  $T_{\text{SDW}}$  and  $T_{\text{SN}}$ , can be considered as a constant. The existing discrepancies with the experimental phase diagram may indicate that a constant  $\alpha$  is not adequate or that another scenario such as orbital nematicity may be more appropriate. Since a rather general form for the spin-fluctuation spectra [see (6)] is employed in our study, the present theory can be applied or extended straightforwardly to other systems where magnetic fluctuations are characterized by four wavevectors with fourfold symmetry. Although cuprate superconductors exhibit nematicity in the magnetic excitation spectra [44] and thus might be possible systems for spin nematic order, the line of onset temperatures of nematicity is nearly parallel to that of the incommensurate magnetic order as a function of doping in  $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}$  [45], which is at variance with figure 8. Instead, the nematicity in cuprates was discussed in terms of a feedback effect from charge nematicity [46, 47].

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